INVESTIGATION OF OPERATING PARAMETERS ON PERFORMANCE AND EMISSION CHARACTERISTICS OF COMPRESSION-IGNITION ENGINES OPERATED BY HYDROGEN AND HYDROGEN-DIESEL MIXTURE

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Registration Number: SVU/PhD/ENGG/ME/002/2021

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THESIS SUBMITTED FOR THE DEGREE OF DOCTOR OF PHILOSOPHY IN MECHANICAL ENGINEERING OF SWAMI VIVEKANANDA UNIVERSITY

2025

ABSTRACT

The global imperative for cleaner energy systems highlights the urgent need to mitigate significant greenhouse gas (GHG) and pollutant emissions, such as particulate matter (PM) and nitrogen oxides (NOx), from conventional diesel engines. Hydrogen-diesel dual-fuel engines emerge as a pivotal advancement, capitalizing on hydrogen's clean combustion properties, zero carbon emissions, high calorific value, rapid flame speed, and wide flammability range, which collectively improve combustion efficiency and reduce PM emissions. This research work aims to comprehensively investigate the performance and emission characteristics of hydrogen-diesel dual-fuel compression-ignition (CI) engines, thereby contributing to a sustainable energy future.

The research adopts a multi-disciplinary approach, integrating detailed experimental investigations with advanced simulation methods. Experimental work has been conducted on a single-cylinder turbocharged diesel engine, with its fuel supply systems and Electronic Control Units (ECUs) modified for dual-fuel combustion. Measurements included in-cylinder pressure, heat release rates, combustion characteristics, and exhaust gas concentrations of hydrocarbons (HC), carbon monoxide (CO), and nitrogen oxides (NOx). Computational simulations has been performed using commercial software, AVL FIRE. These simulations incorporate advanced sub-models for turbulence (modified rapid distortion renormalization group k-ε), chemical kinetics (SAGE and ECFM-3Z models for combustion using n-heptane as a diesel surrogate), NOx formation (extended Zeldovich mechanism), and detailed spray breakup (Kelvin-Helmholtz and Rayleigh-Taylor models). The numerical models validate against experimental data, consistently achieving high correlation coefficients (e.g., R=0.968 for pressure data and R=0.9958 for CO_2 emissions), providing a robust assessment of proposed modifications.

Key findings reveal that hydrogen integration substantially reduces CO_2 and PM emissions, with reductions of up to 90% for PM and 50% for CO_2 through enhanced combustion homogeneity and increased thermal efficiency. However, the elevated combustion temperatures associated with hydrogen often lead to increased NOx emissions. The research demonstrates that optimized Exhaust Gas Recirculation (EGR) rates, precise injection timing, and tailored combustion chamber designs which are crucial for effectively mitigating NOx emissions while simultaneously enhancing thermal efficiency and combustion stability. For instance, up to 88% NOx reduction was achieved with 15% EGR.

Specific optimal hydrogen energy ratios were examined, ranging from 5% to 20%, beyond which volumetric efficiency becomes unaffected and combustion problems may arise. Modifications to the combustion chamber, combined with sac-less injectors, resulted in significant reductions in HC (66.8%), PM (64%), and NOx (30%) in experimental trials. CFD simulations further highlighted that a proposed re-entrant design with increased reentrancy and no central projection could significantly enhance swirl and turbulent kinetic energy (TKE) levels, indicating substantial potential for further emission reductions. Numerical analysis on spray angles revealed that peak cylinder pressure occurred around 140°, while an optimal spray angle range of 120°–160° results to balanced emissions of NOx, unburned methane, and CO, with minimal variation in indicated and combustion efficiencies.

This work significantly advances the development of cleaner, more efficient CI engine technologies, providing critical guidelines for future low-emission engine design and contributing to a sustainable energy future. The novelty of this thesis lies in its detailed assessment of hydrogen-diesel dual-fuel systems, focusing on the interplay of hydrogen-to-diesel mixing ratios, combustion chamber geometry alterations, and the specific quantification of injector spray angle impact on combustion characteristics and emissions.

SUMMERY OF THE RESEARCH WORK

1. INTRODUCTION

This research looks at the prospects of the use of hydrogen as an alternate fuel in a dual-fuel compression-ignition (CI) engine with the objective of curbing the environmental issues posed by the traditional diesel engine. Although diesel engines are well known to be robust, reliable and possess high thermal efficiency, they are also the significant contributors to greenhouse gas (GHG) emissions, particulate matter (PM) and nitrogen oxides (NOx), which have drastic effects on the quality of air, climate change and pose significant threats to human health. The fundamental driving idea behind this study is to find a solution to these urgent environmental issues through the minimization of unwanted emissions, lowering the overall reliance of the world on finite fossil fuels, and utilizing newer technology discoveries in the aspect of hydrogen storage, supply, and injection systems. Moreover, being a zero-carbon energy source, having a high energy concentration and possessing positive combustion characteristic, will make hydrogen an optimal add-on fuel to diesel in a two-way configuration. This method presents a cost effective, technically viable route towards sustainable energy transition that would not require a total restructure of the existing engine infrastructure by incorporating hydrogen into the current CI engines.

2. LITERATURE REVIEW

2.1 Early Developments:

Hydrogen diesel concepts were introduced early in the 20^{th} century, which were enforced during the 1970s oil crisis as a cleaner substitute of diesel. Initial research showed lower particulate matter (PM) and increased performance, but challenges with knocking, backfiring, and the reactivity of hydrogen in particular have hampered their use. In the 1990s, more stable operation became possible with fuel injection and control improving, and two pilot ignition methods improving combustion stability.

2.2 Current Developments:

The new studies use CFD simulation, sophisticated sensors, and material research to create the best hydrogen-diesel burning. Direct hydrogen injection systems reduce the risk of pre-ignition, and allows the optimal control of injection timing, improving efficiency and emissions. Research (Verhelst et al) demonstrates a PM reduction of up to 90 percent and CO_2 reductions of 50 percent. The sustainability is also increased through the use of

renewable hydrogen production through electrolysis. Air-fuel ratios as well as future combustion control is currently optimized by AI-based systems.

2.3 Challenges: Opportunities:

The obstacles are storage infrastructure of hydrogen, safety, and the emission of additional NOx because of the rise in combustion temperature. Exhaust gas recirculation (EGR), water injection are other mitigation strategies, as well as advanced aftertreatment systems. In the improvement of heavy-duty transport, marine, and rail transport, retrofit potential can be used immediately.

2.4 Engine Geometry Role: Key Findings:

The fast flame-speed of hydrogen, low-ignition energy and broad flammability range necessitate such detailing of the combustion chamber geometry, compression ratio, and management of turbulence. The mixing is increased through stepped-lip and re-entrant piston bowls without a lot of knocks. Lean-burn operation with EGR or with water injection can provide important NOx decreases without efficiency penalty, so hydrogen-diesel dual-fuel engines represent an option on the route to low-carbon transport.

2.5 Objective of Present Study

The aim of the current study is to examine the effects of optimized geometry of combustion chamber and enriched diesel fuel with hydrogen on the performance and emission necessities of single-cylinder diesel engine. A modified piston bowl geometry is recommended having an improved reentrancy and lacking the central projection, like the baseline engine it keeps the same compression ratio. The assessments of this geometry are conducted by means of simulations since the end of the suction stroke to the end of the expansion stroke, with the emphasis on the impact of these changes in terms of combustion efficiency and other outcomes in terms of emissions.

3. STATEMENT OF THE PROBLEM

In particular, the below mentioned problem statements will be analyzed in this work:

1. Analysis of combustion chamber geometry on performance of diesel-hydrogen dual-fuel engine

- To model and compare different combustion chamber geometries suitable for diesel–hydrogen dual-fuel operation.

- To evaluate the effects of each geometry on engine performance and exhaust emissions, including NOx, CO, HC.

2. *Numerical analysis of the impact of fuel spray angle on engine performance and emissions.*

- To simulate the combustion process for different spray angles under identical operating conditions.
- To evaluate the influence of spray angle on engine performance and emissions.
- To determine the optimum spray angle that provides a balance between improved performance and reduced emissions.

3. *Experimental analysis of diesel-hydrogen mixture variability on engine performance and emission characteristics.*

- To conduct controlled experimental tests on a single-cylinder diesel engine using each fuel blend.
- To assess performance parameters and exhaust emission characteristics, for different mixture ratios.
- To determine the optimal hydrogen enrichment level that achieves maximum performance with minimal emissions.

3.1 Layout of Thesis

The focus of the present dissertation is associated with study and analyzing the diesel hydrogen dual fuel engine which is expected to be useful for automobile and many other heavy industry sectors. The present work focusses on two of the parameters like, piston geometry design alteration and varying the diesel – hydrogen ratio for combustion to minimize the emission level.

At the beginning, basic modeling of piston bowl geometry is done followed by the numerical analysis using commercial software for different standard and non-standard models. A comparative study and evaluation are performed based on it. Moreover, the mixing ratio of diesel and hydrogen at a constant load condition is tabulated, analyzed and compared.

Chapter one described the background of the research problem to be proposed, giving an introduction. It also outlines the motivation and possible scope of further work on controlling the emission of diesel and hydrogen engine.

Chapter two summarizes the relevant literature on emission control and performance study of diesel hydrogen engine under various situation. In particular, the review is focused on the

study of combustion chamber geometry, mixing ratio of fuels and piston bowl geometry to clearly identify the research gaps.

Chapter three describes analytical and experimental formulation of the problem statement and simulation & analysis of piston chamber geometry to estimate the emission parameter and performance characteristics. In the analysis, a number of variables like – geometrical orientation, mixing ratio of diesel and hydrogen, field of applications etc. has been considered.

Chapter four presents experimental and numerical works using standard methodology. Different phases of trials are discussed here with the help of charts and graphs. Analytical results are compared with the experimental data. The variables are considered based on the standard methodology and realistic load conditions.

Chapter five elaborates the characteristics and comparative analysis of the results obtained from the study (Chapter 4).

Finally, in *chapter six*, conclusions from the present study, major novelty of research work and recommendations for future work are included.

3.2 Contributions of the Thesis

A complete experimental and analytical approach is presented to analyze the performance and emission characteristics for a diesel hydrogen dual fuel engine specific for automobile application. Comprehensive analysis has been performed on designed model with due consideration to the factual working conditions specific to the modified engine model is the main novelty of the work.

In particular, the determination of the optimized mixture of diesel-hydrogen using experimental and numerical analysis can help to reduce the emission. Physical investigation may be used for further phases of trials with different engine models and variable mixing ratios. One of the major findings of the present work is the validation of performance of the conventional system to the predicted model. The comprehensive approach and the results presented in this thesis will help the designers to remodel the hybrid model based on diesel hydrogen system. The present findings are expected to serve as guidelines for various automobile applications.

4. METHODOLOGY

4.1 Engine Model Analysis

The experimental component of this research was carried out on two distinct diesel engine configurations — a single-cylinder, direct-injection diesel engine and a six-cylinder, turbocharged common-rail diesel engine — both modified to operate in hydrogen–diesel dual-fuel mode. Modifications included alterations to the fuel delivery system and reprogramming of the electronic control unit (ECU) to manage dual-fuel injection timing, pulse width, and fuel ratio control. Detailed measurements were recorded, including in-cylinder pressure traces, heat release rates (HRR), and exhaust gas emissions of hydrocarbons (HC), carbon monoxide (CO), and nitrogen oxides (NOx). Testing was performed across varying engine loads and speeds to evaluate combustion stability, thermal efficiency, and pollutant formation under different operating conditions. The experimental data served as a benchmark for assessing the influence of hydrogen substitution levels and injection strategies on both performance and emissions.

4.2 Numerical Investigations

To complement and extend the experimental work, advanced Computational Fluid Dynamics (CFD) simulations were performed using AVL FIRE and CONVERGE CFD software platforms. The numerical analysis aimed to optimize piston bowl geometry, hydrogen substitution ratios, and fuel injection parameters for enhanced performance and reduced emissions. The simulations incorporated RNG k–ε turbulence models for accurate turbulence prediction, SAGE and ECFM-3Z combustion models for detailed combustion kinetics, and the extended Zeldovich mechanism for precise NOx formation analysis. Spray breakup and evaporation processes were modelled using KH–RT and Frossling correlations, ensuring realistic representation of fuel–air mixing. Extensive model validation against experimental results was carried out to ensure reliability, enabling the simulations to provide detailed insights into flame propagation, heat release characteristics, and pollutant formation mechanisms.

5. RESULTS AND DISCUSSION

5.1 Experimental Results

Experimental investigations on both single-cylinder and six-cylinder CI engines revealed that hydrogen substitution led to substantial improvements in brake thermal efficiency

(BTE) and a marked reduction in CO_2, soot, and particulate matter emissions**.** The optimal hydrogen-to-diesel energy share was found to be within 15–25%, balancing efficiency gains with combustion stability. Exhaust Gas Recirculation (EGR) effectively reduced NOx emissions without severely compromising performance.

5.2 Numerical Simulation Outcomes

Software simulations in AVL FIRE validates the experimental results, enabling detailed analysis of spray atomization, in-cylinder turbulence, and flame propagation. Optimized piston bowl geometries—specifically re-entrant designs without central projections—enhanced air–fuel mixing, resulting in improved combustion efficiency and lower HC emissions.

5.3 Comparative Analysis and Discussion

Comparative analysis confirmed that combining chamber geometry optimization with hydrogen substitution achieved the best trade-off between performance and emissions. Numerical results closely matched experimental data, with deviations under 5%, confirming model reliability. The integration of spray dynamics modelling with hydrogen blending strategies demonstrated a scalable approach for future CI engine designs. This combined methodology provides a robust foundation for developing low-emission, high-efficiency hydrogen–diesel engines.

6. CONCLUSIONS

The thesis examines diesel and hydrogen in compression ignition (CI) engines encompassing hydrogen-diesel, dual-fuel systems with respect to hydrogen blend ratios and injector spray angles in the combustion chamber. The outcomes confirm that the addition of hydrogen increases the thermal efficiency, cylinder pressure, heat release rates, reduces the code content, PM content, and HC emissions. Nevertheless, the high hydrogen levels restrict the oxygen availability and hence promotes incomplete combustion and high levels of CO emissions, and the high temperatures of the combustion process promote high levels of NOx, which can be controlled by EGR. The efficiency and emissions are balanced (with no trade-off on combustion stability) and an optimal hydrogen substitution range of 5-20 percent is found. The shape of the combustion chambers has emerged to be a major issue in consideration to cater to the specification of hydrogen.

Experiments are used, and their results are complemented with CFD numerical simulations, which offer a high level of information regarding the spray dynamics, reaction timing, among

other factors. Variation in spray angle analysis indicates that rising the spray angle range in study variables to 140^{o} as opposed to 60^{o} enhances peak cylinder pressure, combustion efficiency and decrease in CO and methane emission. Nevertheless, overspray angles incur efficiency loss and high emissions of NOx. The ideal range (120^{o} to 160^{o}) of the spray angle alters the reduction of CO, unburned methane, and NOx to an optimal level.

On the whole, it should be emphasized, that the experimental analysis and CFD-based optimization of hydrogen-diesel dual-fuel engines can be considered to contribute to the development of cleaner, more efficient, sustainable alternative propulsion technologies.

6.1 Novelty of Work:

The novelty of the work can be identified from two distinct studies:

- The research determines the influence of varying spray angles (from 60° to 160°) on several key parameters, including peak cylinder pressure, start of combustion (SOC), crank angle at 50% combustion (CA50), duration of combustion, average in-cylinder temperature, NOx emissions, unburned methane emissions, and carbon monoxide (CO) emissions.
- This study reveals some valuable insights into the complex interactions between spray angle, combustion dynamics, and emissions characteristics in NG-diesel dual-fuel engines.
- An optimal spray angle range of 120° to 160° has been determined in this study to achieve a balance among NOx, unburned methane, and CO emissions.

6.2 Future Scopes

- **Optimization of Hydrogen-Diesel Ratio and Fuel Management Strategies:** Future research should be performed to develop adaptive control and machine learning algorithms to optimize hydrogen-diesel ratios under dynamic loads, improving combustion stability, drivability, efficiency, and emissions beyond the current 5–20% hydrogen energy range.
- **Extensive Parametric Studies and AI-driven Optimization for Combustion Chamber Design:** Future research should include CFD and AI-based optimization to evaluate diverse piston bowl geometries, aiming to minimize knock and thermal stress under high hydrogen use and optimize combustion across injection strategies.
- **Development of Adaptive and Advanced Fuel Injection Systems:** Future study should be performed to develop adaptive spray systems and multi-pattern injectors to improve air- fuel mixing, while advanced injection strategies like split and post-injection can

reduce knock and NOx under hydrogen-rich conditions.

- **Adoption of a Multi-disciplinary Approach and Exploration of Hybrid Fuel Systems:** Future research should be focused on a multi-disciplinary approach, combining combustion science, controls, and materials, with a focus on hybrid fuels like hydrogen, CNG, and diesel for commercial viability.

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7. Performance and Emission Characteristics of a Hydrogen-Diesel Dual Fuel Engine under Variable Load Conditions, 1st International Conference on Sustainable Research and Development (ICSRD) 2024, 25th & 26th September, 2024

(12) PATENT APPLICATION PUBLICATION

(19) INDIA

(22) Date of filing of Application :12/03/2025

(21) Application No.202531022103 A

(43) Publication Date : 28/03/2025

(54) Title of the invention : Piston bowl for a dual-fuel hydrogen-diesel engine

(51) International classification :F02F3/26, F02B23/06, F02F3/28, F02B23/10, F02B 23/00
(86) International Application No :NA
Filing Date :NA
(87) International Publication No : NA
(61) Patent of Addition to Application Number :NA
Filing Date :NA
(62) Divisional to Application Number :NA
Filing Date :NA

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(57) Abstract :
The present invention relates to an advanced piston bowl design for dual-fuel hydrogen-diesel engines, optimized to enhance combustion efficiency, emission control, and thermal management. The piston bowl integrates micro-channels for controlled hydrogen injection, radial grooves for enhanced air-fuel mixing, and an asymmetric curvature for stratified charge combustion. A stepped-lip structure ensures stable flame propagation, reducing knocking and abnormal combustion. The design includes dedicated regions for diesel pilot ignition and hydrogen-air premixing, preventing pre-ignition and ensuring precise combustion phasing. An adaptive wall thickness scheme improves heat dissipation, enhancing durability under high-temperature conditions. By optimizing fuel-air mixing, ignition timing, and flame control, the invention significantly reduces NOx emissions, improves fuel efficiency, and extends engine lifespan, making hydrogen-diesel dual-fuel technology more viable for sustainable applications.

No. of Pages : 15 No. of Claims : 8